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AUTHOR(S):

OHKAWA, Fusayoshi J.; FUKUYAMA, Hidetoshi;
YOSIDA, Kei

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Kondo Effect and Localization in Two-Dimensional Systems

Fusayoshi J. OHKAWA, Hidetoshi FUKUYAMA and Kei YOSIDA

Institute for Solid State Physics
The University of Tokyo

1. Kondo Effect

Interplay between localization and the Kondo effect is discussed in a two-dimensional system.¹⁻³⁾ Various physical quantities are calculated perturbatively in terms of exchange coupling constant J and $\lambda = \pi/2\pi\epsilon_F\tau_0$ where ϵ_F is the Fermi energy and τ_0 is the relaxation time of plane wave states. There are two physical parameters characterizing the present system. One is the Kondo temperature kT_K , and the other is a typical localization energy given by $\pi\omega_L = (\pi/\tau_0)\exp(-1/2\lambda)$. Theoretical analysis is reliable for small λ ($\lambda \ll 1$). Therefore we will confine ourselves to the case $\lambda \ll 1$, and $kT_K \gg \pi\omega_L$. Perturbative calculations presented in the following are valid at high temperatures such as $kT \gg kT_K \gg \pi\omega_L$. We assume that $J_x = J_y$.

The susceptibility is calculated as

$$\chi = \chi_0 \left[1 + 4J_x^2 X(T) + O(J_x J_y J_z) \right], \quad (1)$$

where $\chi_0 = (g\mu_B)^2/4$ is that of a free spin, and quantity $X(T)$ is given by

$$X(T) = \int d\epsilon_1 \int d\epsilon_2 g_2(\epsilon_1, \epsilon_2) \frac{f(\epsilon_1) - f(\epsilon_2)}{(\epsilon_1 - \epsilon_2)^2} \left[1 + \frac{1}{\beta(\epsilon_1 - \epsilon_2)} \right], \quad (2)$$

Here $g_2(\epsilon_1, \epsilon_2)$ is the ensemble average of local densities of states defined by

$$g_n(\epsilon_1, \epsilon_2, \dots, \epsilon_n) = \langle\langle \frac{1}{\Omega} \int dr \rho(\epsilon_1, r) \rho(\epsilon_2, r) \dots \rho(\epsilon_n, r) \rangle\rangle, \quad (3)$$

where $\rho(\epsilon)$ is the local density of state at r in the presence of disorder. When a perturbative result (given by eq.(6)) is used for g_2 , $X(T)$ is calculated as

$$X(T) = \rho_0^2 \left[\ln(\epsilon_F/kT) + \lambda \ln^2(\pi/2\pi\tau_0 kT) + O(\lambda^2) \right]. \quad (4)$$

The first term in eq.(4) is the well known Kondo logarithmic term for clean systems. Here a more singular term is obtained. The relaxation time of plane wave states due to paramagnetic impurities is calculated as

$$\frac{\pi}{2\tau_s} = n_s \pi \rho_0 \left\{ \frac{1}{4} (2J_x^2 + J_z^2) - 3\rho_0 J_x^2 J_z \left[\ln\left(\frac{\epsilon_F}{kT}\right) + \frac{\lambda \pi \pi}{6\tau_0 kT} + O(\lambda^2) \right] + O(J^4) \right\}. \quad (5)$$

In the case of electron-electron interaction, the quantum correction is proportional to $\ln T$. In the present case, a more singular term, $1/T$, is present.

Let us investigate the general structure of the susceptibility expansion in terms of the exchange coupling constant. When g_n is introduced, the formal structures of the expansion are exactly the same in both clean and disordered systems in every order of J although g_n may be different in both cases. The effect of localization can, thus, be expressed through g_n . On the other hand,

finite density of states for local infinitesimally small excitations of electron-hole pairs across the Fermi level is indispensable for the realization of the Kondo effect. This condition is identical to finite g_n in the limit of equal energies ($\varepsilon_1 \rightarrow \varepsilon_F$) for any n .

In the following, it will be shown that $g_2(\varepsilon_F, \varepsilon \rightarrow \varepsilon_F)$ is non zero. If there exists a critical n_c , i.e., if g_n vanishes for $n \geq n_c$, then n_c is expected to be 2 or ∞ . Because a possibility of $n_c=2$ is denied there, it can be expected that g_n is also non zero for any finite n , and that the ground states is qualitatively the same as in pure systems; the ground states is singlet for anisotropy $|J_x| > J_z$, and Ising-like doublet for anisotropy $|J_x| \leq J_z$. In either case, paramagnetic impurities do not destroy localization.

2. Local Density of States, $g_2(\varepsilon, \varepsilon + \pi\omega)$

Quantity g_2 is discussed here.^{3,4)} The self-consistent theory due to Vollhardt and Wölfle⁵⁾ gives

$$\begin{aligned} g_2(\varepsilon, \varepsilon + \pi\omega) &= \rho_0^2 \left[1 - 2\lambda \ln(\omega\tau) + O(\lambda^2) \right] \text{ for } \omega \gg \omega_L \\ &= \rho_0^2 (2/\lambda - 1) \text{ for } \omega < \omega_L. \end{aligned} \quad (6)$$

The self-consistent theory reproduces the perturbational result for $\omega \gg \omega_L$, and it predicts that g_2 does not vanish in the limit of equal energies. Here it becomes clear what the localization energy means. When the frequency is as low as the localization energy, the term proportional to λ becomes of the order of unity; the perturbational calculation becomes wrong in such a low frequency regime. This is a definition of the localization energy here.

However it is generally understood that the self-consistent theory does not include the effect of the so called "level repulsion". Therefore it is necessary to investigate g_2 by including "level repulsion".⁶⁾ Then

$$\begin{aligned} g_2(\varepsilon, \varepsilon + \pi\omega) &\propto |\ln^{d-1}(\omega\tau)| \\ \lim_{q \rightarrow 0} \sigma(\pi\omega + i0; q) &\propto \omega |\ln^{d+1}(\omega\tau)|, \end{aligned} \quad (7)$$

for small ω . The logarithmic dependence of the conductivity has already been discussed by Mott⁶⁾.

The following physical picture of localization is implicitly assumed in the level repulsion mechanism;⁴⁾ every eigenfunction is determined by a Schrödinger equation, which has no real space symmetries in disordered systems. Only the parameter in the equation is the energy. Therefore it is a reasonable expectation that two states whose eigenvalues are very close to each other must behave similarly. The expectation is the case in a certain sense even if the states are localized. When the level repulsion occurs, the linear combinations are formed between two states far in space. These two states behave similarly to each other. Otherwise they behave differently, even if their eigenvalues are close to each other. When the level repulsion is significant, the envelope of eigenfunctions is like a group of islands scattered in the ocean; each "island" is exponentially

decayed. The true eigenstates are linear combinations of "islands".

Orthogonalization between two states having large amplitudes in the same regions are possible in two manners. One manner of orthogonalization is local; the two states have different number of nodes within a single exponential decay region, and they are nearly orthogonal locally to each other. They can not be close to each other in this case. A typical energy for this repulsion is the localization energy. For example, let us consider a finite extended system whose linear dimension is about ξ , and assume that the two states lie around the Fermi level and that they have n and $n+1$ nodes, respectively, along one direction; the profiles along the other directions are similar. The difference of their energies is given by

$$\Delta E = \frac{\hbar^2}{2m\xi^2} [(n+1)^2 - n^2] \simeq \frac{\hbar^2 n}{m\xi^2} \longrightarrow \hbar\omega_L. \quad (8)$$

In two dimensional systems, eq.(8) gives $\hbar\omega_L$ if we take $n = k_F \xi$, and the localization length as ξ given in ref 7); k_F is the Fermi wave vector. As far as the frequency dependences of $\sigma(\omega)$ and $g_2(\xi, \xi + \hbar\omega)$ are concerned in the region of frequency much larger than the localization energy, the system behaves like extended systems; the conductivity has a Drude tail and g_2 is nearly constant in such a region. Such a region is nothing but the weakly localized regime. The other manner of orthogonalization is possible. The two states have the same number of nodes locally within their exponential decay regions, i.e., within "islands", but their phases are different among "islands". In this latter case, the two states can be infinitesimally close to each other. Those pairs contribute to the logarithmic dependence of the conductivity and g_2 in very low frequency. This low frequency regime is the strongly localized regime.

Finally we should mention that it is very interesting to examine g_2 and the conductivity by a more precise treatment; especially it is the most interesting to examine whether the divergence in g_2 still remains or not in dimensions higher than one.

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